Chapter 2

Coupling of angular momenta

2.1 Definitions

Consider the operator J defined by

$$J = J_1 + J_2 \tag{2.1}$$

The two operators on the left hand side act on different systems (1 and 2) and do therefore commute, *c.f.* $J_1 = L$ and $J_2 = S$. J is an angular momentum because the operator obey the commutation relation Eq. (1.4),

$$\begin{aligned}
[J_i, J_j] &= [J_{1i} + J_{2i}, J_{1j} + J_{2j}] = [J_{1i}, J_{1j}] + [J_{1i}, J_{2j}] + [J_{2i}, J_{1j}] + [J_{2i}, J_{2j}] \\
&= i\hbar\epsilon_{ijk}J_{1k} + i\hbar\epsilon_{ijk}J_{2k} = i\hbar\epsilon_{ijk}J_k
\end{aligned}$$

Because J_1 and J_2 commute, J_1^2, J_2^2, J_{1z} and J_{2z} all commute and the simultaneous eigenfunctions make up a complete basis. We note that the operator Γ with quantum number γ sometimes has to be introduced to make the basis truly complete, *i.e.* the situation could arise where the eigenfunctions are not uniquely specified by other quantum numbers. An example of this situation is the double occurrence of the terms ${}^2D$, ${}^2F$, ${}^2G$ and ${}^2H$ in the $4f^3$ and $4f^{11}$ configurations (Nd^{3+} and Er^{3+}) and the ten times occurring ${}^2F$ and ${}^2G$ terms in $4f^7$ of Gd^{3+}. Without the extra quantum numbers that γ represent (in these cases $\gamma = \nu(w_1w_2w_3)(u_1u_2)$ [1]) we could not differentiate between the states. It was of course Racah that solved these difficulties in his papers [7,8]. The simultaneous eigenkets to the observables Γ, J_1^2, J_2^2, J_{1z} and J_{2z} are written

$$|\gamma j_1 j_2 m_1 m_2\rangle \tag{2.2}$$

These kets are the so called basis kets for the m_1m_2- representation.

We showed above that J defined by Eq. (2.1) was an angular momentum operator. Because Γ, J^2, J_z, J_1^2 and J_2^2 all commute the simultaneous eigenkets

$$|\gamma j_1 j_2 JM\rangle \tag{2.3}$$

[1] As we will see later, group theory played an important role in Racahs work. Actually, on restricting a group of transformations to its sub-groups (in the case of $4f^n$, $R_3 \subset G_2 \subset R_7 \subset SU_7 \subset U_7 \subset GL_7$) the irreducible representation of the group decompose into the irreducible representations of the sub-groups.

will also form a complete system. These eigenkets are the basis kets for the JM-representation.

2.2 Re-coupling of two angular momenta, Clebsch-Gordan coefficients

The two systems with eigenkets Eqs. (2.2) and (2.3) are orthonormal which mean that we have a unitary transformation between the two systems. The transformation can be written

$$|\gamma j_1 j_2 JM\rangle = \sum_{\gamma' j_1' j_2' m_1' m_2'} |\gamma' j_1' j_2' m_1' m_2'\rangle\langle\gamma' j_1' j_2' m_1' m_2'|\gamma j_1 j_2 JM\rangle \tag{2.4}$$

The expansion coefficients $\langle\gamma' j_1' j_2' m_1' m_2'|j_1 j_2 JM\rangle$ (overlap) is the scalar product between the two functions

$$\langle\gamma' j_1' j_2' m_1' m_2'|\gamma j_1 j_2 JM\rangle = \int d\bar{r}\Psi^*(\gamma' j_1' j_2' m_1' m_2')\Phi(\gamma j_1 j_2 JM) \tag{2.5}$$

Note that we have used

$$1 = \sum_{\gamma' j_1' j_2' m_1' m_2'} |\gamma' j_1' j_2' m_1' m_2'\rangle\langle\gamma' j_1' j_2' m_1' m_2'| \tag{2.6}$$

in Eq. (2.4). The scalar product Eq. (2.5) is independent of γ and non-zero only if $j_1' = j_1$, $j_2' = j_2$ and $m_1 + m_2 = M$. This simplifies Eq. (2.4) to

$$|\gamma j_1 j_2 JM\rangle = \sum_{m_1+m_2=M} |\gamma j_1 j_2 m_1 m_2\rangle\langle j_1 j_2 m_1 m_2|j_1 j_2 JM\rangle \tag{2.7}$$

To prove that Eq. (2.5) vanish unless $m_1 + m_2 = M$ we note that $(J_z = J_{1z} + J_{2z})$

$$(J_z - J_{1z} - J_{2z})|j_1 j_2 JM\rangle = 0. \tag{2.8}$$

Multiply from the left with the bra $\langle j_1 j_2 m_1 m_2|$, and we get

$$(M - m_1 - m_2)\langle j_1 j_2 m_1 m_2|j_1 j_2 JM\rangle = 0 \tag{2.9}$$

Obviously $M = m_1 + m_2$ if $\langle j_1 j_2 m_1 m_2|j_1 j_2 JM\rangle \neq 0$ The next thing to note is that the coefficients vanish unless $J = |j_1 - j_2|, |j_1 - j_2| + 1, \ldots, j_1 + j_2$. This is most easily shown by checking that the dimensionality is the same for both spaces, spanned by $\{|j_1 j_2 m_1 m_2\rangle\}$ and $\{|j_1 j_2 JM\rangle\}$, respectively. In the $m_1 m_2$-representation we have $N_1 = (2j_1+1)(2j_2+1)$ because the possible values of M is $-J, \ldots, J$ (see Eq. (1.24)). The dimensionality of the space in the JM-representation is straight forward to derive by assuming that J runs from $j_1 - j_2$ to $j_1 + j_2$ $(j_1 \geq j_2)$. For each J we have $2J + 1$ states. Adding we get

$$\begin{aligned} N_2 &= \sum_{j=j_1-j_2}^{j=j_1+j_2} (2J+1) = [\text{Gauss formula}] = \\ &= \frac{1}{2}(2(j_1 - j_2) + 1 + 2(j_1 + j_2) + 1)(2j_2 + 1) = (2j_1 + 1)(2j_2 + 1) \end{aligned}$$

Thus, we see that $N_1 = N_2$ if $J = |j_1 - j_2|, |j_1 - j_2| + 1, \ldots, j_2 + j_2$. Corresponding to Eq. (2.7) we have

$$|\gamma j_1 j_2 m_1 m_2\rangle = \sum_{j=|j_1-j_2|}^{j=j_1+j_2} |\gamma j_1 j_2 JM\rangle\langle j_1 j_2 JM|j_1 j_2 m_1 m_2\rangle \tag{2.10}$$

and directly from Eq. (2.5) we have

$$\langle j_1 j_2 JM|j_1 j_2 m_1 m_2\rangle = \langle j_1 j_2 m_1 m_2|j_1 j_2 JM\rangle^* \tag{2.11}$$

Next, two very useful orthogonality relations will be proven. These are:

i) $$\sum_{m_1 m_2} \langle j_1 j_2 m_1 m_2|j_1 j_2 JM\rangle\langle j_1 j_2 J'M'|j_1 j_2 m_1 m_2\rangle = \delta_{J'J}\delta_{M'M}$$

ii) $$\sum_{JM}\langle j_1 j_2 JM|j_1 j_2 m_1 m_2\rangle\langle j_1 j_2 m_1' m_2'|j_1 j_2 JM\rangle = \delta_{m_1' m_1}\delta_{m_2' m_2}$$

The proof for i) is obtained by starting with

$$\langle j_1 j_2 J'M'|j_1 j_2 JM\rangle = \delta_{J'J}\delta_{M'M},$$

inserting a "1" (closure)

$$\sum_{j_1' j_2' m_1 m_2} |j_1' j_2' m_1 m_2\rangle\langle j_1' j_2' m_1 m_2| = 1$$

and we have proven the equality

$$\sum_{m_1 m_2} \langle j_1 j_2 J'M'|j_1 j_2 m_1 m_2\rangle\langle j_1 j_2 m_1 m_2|j_1 j_2 JM\rangle = \delta_{J'J}\delta_{M'M} \tag{2.12}$$

The next proof is equally trivial

$$\langle j_1 j_2 m_1' m_2'|j_1 j_2 m_1 m_2\rangle = \delta_{m_1' m_1}\delta_{m_2' m_2}$$

and once again inserting a "1" (closure)

$$\sum_{j_1' j_2' JM} |j_1' j_2' JM\rangle\langle j_1' j_2' JM| = 1$$

which give us the proof

$$\sum_{JM}\langle j_1 j_2 m_1' m_2'|j_1 j_2 JM\rangle\langle j_1 j_2 JM|j_1 j_2 m_1 m_2\rangle = \delta_{m_1' m_1}\delta_{m_2' m_2} \tag{2.13}$$

2.2.1 The Clebsch-Gordan coefficients

The coefficients discussed in section 2.2 are of course the Clebsch-Gordan coefficients $\langle j_1 j_2 m_1 m_2 | j_1 j_2 J M\rangle$. These coefficients are non-zero only if

$$\left.\begin{array}{rcl} m_1 &=& -j_1, \ldots, j_1 \\ m_2 &=& -j_2, \ldots, j_2 \\ M &=& m_1 + m_2 = -J, \ldots, J \\ J &=& |j_1 - j_2|, \ldots, j_1 + j_2 \end{array}\right\}$$

The Clebsch-Gordan coefficients are simply the elements of a matrix that connect the $\{m_1 m_2\}$-basis with the $\{JM\}$-basis. We will return to these coefficients (derive recursion relations) later on.

2.2.2 The phase convention of Condon & Shortley

Every wave function has a phase associated to it. The phase is of course arbitrary because only the square of the wave function has physical significance. However, the phase has to be fixed and kept throughout the calculations. It is common to use the phase conventions introduced in the book of Condon & Shortley [4]. The convention follows:

I) $J_\pm$ only change m with $\pm\hbar$ and leave the other quantum numbers unchanged. The first phase convention define the matrix elements of these operators to be real and positive, *i.e.* the phase between two wave functions that only differ in m is now fixed.

II) $|\gamma j_1 j_2 (j_1 + j_2)(j_1 + j_2)\rangle = |\gamma j_1 j_2 j_1 j_2\rangle$. The phase between the basis kets of the two systems. Note that the left hand side ket has $J = j_1 + j_2$ and $M = j_1 + j_2$ and that the ket on the right hand side has $m_1 = j_1$ and $m_2 = j_2$.

III) All non-diagonal matrix elements of J_{1z} are real and non-negative. This fix the phase for the wave functions with different j ($\Delta j = 1$).

2.3 The Wigner 3j-symbol

Using the different commutation relations derived so far and the phase conventions in the previous section, it is possible to derive an algebraic expression for the Clebsch-Gordan coefficients. This is very tedious and we therefore only give the final expression (see for example Eq. (16) in Racah [3]).

$$\begin{aligned} &\langle j_1 j_2 m_1 m_2 | j_1 j_2 J M\rangle = \delta_{m_1+m_2,M} \\ \times\ & \left[\frac{(2J+1)(j_1+j_2-J)!(j_1-m_1)!(j_2-m_2)!(J+M)!(J-M)!}{(j_1+j_2+J+1)!(J+j_1-j_2)!(J+j_2-j_1)!(j_1-+m_1)!(j_2+m_2)!}\right]^{1/2} \\ \times\ & \sum_x (-1)^{j_1-m_1-x} \frac{(j_1+m_1+x)!(j_2+J-m_1-x)!}{x!(J-M-x)!(j_1-m_1-x)!(j_2-J+m_1+x)!} \end{aligned} \tag{2.14}$$

This expression is obviously :) very symmetric, *e.g.* with $x = J - M - y$, we get

$$\langle j_1 j_2 m_1 m_2 | j_1 j_2 J M\rangle = (-1)^{j_1+j_2-J}\langle j_2 j_1 m_2 m_1 | j_2 j_1 J M\rangle \tag{2.15}$$

The important conclusion is that the Clebsch-Gordan coefficients are not symmetric with respect to the three angular momenta j_1, j_2 and J.

In 1951 Wigner [5] introduced the $3j$-symbol, defined by

$$\begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix} = (-1)^{j_1-j_2-m_3}(2j_3+1)^{-1/2}\langle j_1 j_2 m_1 m_2 | j_1 j_2 j_3 - m_3\rangle \tag{2.16}$$

The $3j$-symbol was designed to display symmetries such as Eq. (2.15) in a symmetric and uniform way. For example, an odd number of permutations of the columns change sign if $j_1 + j_2 + j_3$ is odd, *i.e.*

$$\begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix} = (-1)^{j_1+j_2+j_3}\begin{pmatrix} j_2 & j_1 & j_3 \\ m_2 & m_1 & m_3 \end{pmatrix} \tag{2.17}$$

whereas an even permutation do not change sign

$$\begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix} = \begin{pmatrix} j_2 & j_3 & j_1 \\ m_2 & m_3 & m_1 \end{pmatrix} \tag{2.18}$$

It also follows that $3j$-symbols with two identical columns are zero, and it can be shown that

$$\begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix} = (-1)^{j_1+j_2+j_3}\begin{pmatrix} j_1 & j_2 & j_3 \\ -m_1 & -m_2 & -m_3 \end{pmatrix} \tag{2.19}$$

Analogous orthogonality relations to those for the Clebsch-Gordan coefficients Eqs. (2.12) and (2.13) will now be derived.

i) $$\sum_{m_1 m_2}\begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix}\begin{pmatrix} j_1 & j_2 & j_3' \\ m_1 & m_2 & m_3' \end{pmatrix} = \frac{\delta_{j_3' j_3}\delta_{m_3' m_3}}{[j_3]} \tag{2.20}$$

ii) $$\sum_{m_1 m_2 m_3' m_3}\begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix}\begin{pmatrix} j_1 & j_2 & j_3' \\ m_1 & m_2 & m_3' \end{pmatrix} =$$

$$\sum_{m_1 m_2 m_3}\begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix}\begin{pmatrix} j_1 & j_2 & j_3' \\ m_1 & m_2 & m_3 \end{pmatrix} = \delta_{j_3' j_3} \tag{2.21}$$

ii) $$\sum_{j_3 m_3}\begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix}\begin{pmatrix} j_1 & j_2 & j_3 \\ m_1' & m_2' & m_3 \end{pmatrix}(2j_3+1) = \delta_{m_1' m_1}\delta_{m_2' m_2} \tag{2.22}$$

Eq. (2.16) relate the $3j$-symbol with the Clebsch-Gordan coefficients and Eqs. (2.12) and (2.13) are the orthogonality conditions. The proof of i) is straight forward, Eqs (2.12), (2.16) and (2.11) immediately give

$$\sum_{m_1 m_2}\begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & -m_3 \end{pmatrix}(-1)^{-j_1+j_2-m_3}(2j_3+1)^{1/2}\begin{pmatrix} j_1 & j_2 & j_3' \\ m_1 & m_2 & -m_3' \end{pmatrix}\times$$
$$(-1)^{-j_1+j_2-m_3'}(2j_3'+1)^{1/2} = \delta_{j_3' j_3}\delta_{m_3' m_3}$$

Noting that the sum is independent of j_1, j_2 and m_3 plus the variable substitutions $-m_3 \to m_3$ and $-m_3' \to m_3'$ proves the equality. The second proof we obtain by noting that the first equality comes from $\delta_{m_3' m_3}$ in i). The second equality comes from the fact that there are $(2j_3+1)$ m_3 states. Now using the results of i) we have proven ii). The last proof iii) is very similar to that of i). Eqs (2.13), (2.16) and (2.11) result in

$$\sum_{j_3 m_3} \begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & -m_3 \end{pmatrix} (-1)^{-j_1+j_2-m_3}(2j_3+1)^{1/2} \begin{pmatrix} j_1 & j_2 & j_3 \\ m_1' & m_2' & -m_3 \end{pmatrix} \times$$
$$(-1)^{-j_1+j_2-m_3}(2j_3+1)^{1/2} = \delta_{m_1' m_1}\delta_{m_2' m_2}$$

By substituting $-m_3 \to m_3$ we arrive at the desired result.

The $3j$-symbols are non-zero only if

$$\left.\begin{array}{l} m_i = -j_i, \ldots, j_i \\ m_1 + m_2 + m_3 = 0 \\ |j_1 - j_2| \leq j_3 \leq j_1 + j_2 \end{array}\right\}$$

which is obvious because the Wigner $3j$-symbol is proportional to the Clebsch-Gordan coefficients, *c.f.* Eqs. (2.16) and (2.14). There are many special cases where the evaluation of the $3j$-symbols is particularly simple. One such case is

$$\begin{pmatrix} j & j & 0 \\ m & -m & 0 \end{pmatrix} = (-1)^{j-m}(2j+1)^{-1/2} \tag{2.23}$$

Wigner's definition of the $3j$-symbol is not the only work on symmetriesed coefficients. Below is a table including four other symmetriesed coefficients and their relation to the Wigner $3j$-symbol.

Racah(1942) $$\mathrm{V}(j_1 j_2 j_3; m_1 m_2 m_3) = (-1)^{j_3+j_2-j_1} \begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix} \tag{2.24}$$

Landau & Lifschitz(1948) $$\mathrm{S}_{j_1 m_1; j_2 m_2; j_3 m_3} = (-1)^{j_1-j_2+j_3} \begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix} \tag{2.25}$$

Fano(1952) $$\langle j_1 m_1, j_2 m_2, j_3 m_3 | 0 \rangle = (-1)^{j_1+j_2+j_3} \begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix} \tag{2.26}$$

Schwinger(1952) $$\mathrm{X}(j_1 j_2 j_3; m_1 m_2 m_3) = \begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix} \tag{2.27}$$

These symmetriesed coefficients are being used less and less often and the Wigner $3j$-symbol seem to be the one surviving.

2.4 Coupling and re-coupling of 3, 4 and 5 angular momenta; 6j-, 9j- and 12j-symbols

In the previous section we did see how the $3j$-symbol came about when investigating the re-coupling of two angular momenta. We will now see that the same reasoning as used above can be generalized to include an arbitrary number of angular momenta. When studying the re-coupling of 3, 4 and 5 angular momenta we will see that the $6j$-, $9j$- and $12j$-symbols will appear rather naturally in this process. There is one more obvious difference when re-coupling more than two angular momenta compared to the re-coupling of two angular momenta, we have to specify intermediate states, and this will result in a rather "messy" index "orgy" as will be apparent in the next sections. The short notation $[x] = (2x+1)$ will continue to be used extensively.

2.4.1 The 6j-symbol

Consider the coupling of three angular momenta j_1, j_2 and j_3, forming the resultant J. We start with the eigenkets

$$|\gamma j_1 j_2 j_3 m_1 m_2 m_3\rangle \tag{2.28}$$

of $\Gamma, J_1^2, J_2^2, J_3^2, J_{1z}, J_{2z}$ and J_{3z}. A first naive attempt to form an eigenket including J would be $|\gamma j_1 j_2 j_3 JM\rangle$ of $\Gamma, J_1^2, J_2^2, J_3^2, J^2, J_z$, but as we will show, γ, j_1, j_2, j_3, J and M do not uniquely define the states, *i.e.* more then one eigenfunction will have the same J and M. To see that our naive attempt fails we perform a dimensional analysis. Eq. (2.28) have the dimension

$$(2j_1+1)(2j_2+1)(2j_3+1) \tag{2.29}$$

for obvious reasons. $|\gamma j_1 j_2 j_3 JM\rangle$ has the dimension (in the best case where we assume the summation start from 0)

$$\begin{aligned}\sum_{J=0}^{j_1+j_2+j_3}(2J+1) &= \frac{1}{2}(2(j_1+j_2+j_3)+1+1)(j_1+j_2+j_3+1)\\ &= (j_1+j_2+j_3+1)^2 \end{aligned}\tag{2.30}$$

With $j_1 = j_2 = j_3 = 1$ (just as an example) we get 27 and 16 for the two different expressions. Obviously it is not correct to just add the three angular momenta forming J. Giving it a little extra thought one realize that because $|\gamma j_1 j_2 j_3 m_1 m_2 m_3\rangle$ and $|\gamma j_1 j_2 j_3 JM\rangle$ do not even have the same number of quantum numbers, something must be done. The solution is to specify an intermediate state j_{12}, j_{23} or j_{13}. Choosing j_{12} we get the dimension

$$\begin{aligned}\sum_{j_{12}=j_1-j_2}^{j_1+j_2}\sum_{J=j_{12}-j_3}^{j_{12}+j_3}(2J+1) &= \sum_{j_{12}=j_1-j_2}^{j_1+j_2}(2j_{12}+1)(2j_3+1)\\ &= (2j_1+1)(2j_2+1)(2j_3+1)\end{aligned}\tag{2.31}$$

which obviously is in agreement Eq. (2.29). In analogy with the standard addition of vectors, our next attempt (which of course will be successful) will be to additionally specify an intermediate resultant, *i.e.* including the eigenstates of J_{12}^2, J_{23}^2 or J_{13}^2. The eigenkets now takes the form (for the two first choices)

$$|\gamma(j_1 j_2) j_{12} j_3 JM\rangle \tag{2.32}$$

or

$$|\gamma j_1 (j_2 j_3) j_{23} JM\rangle \tag{2.33}$$

Both sets of quantum numbers uniquely specify the states. Note that

$$\left.\begin{array}{rcl} j_{12} & = & |j_1 - j_2|, \ldots, j_1 + j_2 \\ j_{23} & = & |j_2 - j_3|, \ldots, j_2 + j_3 \end{array}\right\} \tag{2.34}$$

The two different coupling schemes can be visualized in with help from figure **??**.
fig2.

Similar to the case where we coupled two angular momenta we can change between the two representation, *c.f.* Eq. (2.7).

$$\begin{aligned} |\gamma(j_1 j_2) j_{12} j_3 JM\rangle = & \sum_{m_{12} m_3} |\gamma(j_1 j_2) j_{12} j_3 m_{12} m_3\rangle \times \\ & \langle\gamma(j_1 j_2) j_{12} j_3 m_{12} m_3 | \gamma j_1 (j_2 j_3) j_{23} JM\rangle \end{aligned} \tag{2.35}$$

The ket on the right hand side of Eq. (2.35) can be decoupled,

$$|\gamma j_1 j_2 j_{12} m_{12}\rangle = \sum_{m_1 m_2} |j_1 j_2 m_1 m_2\rangle \langle j_1 j_2 m_1 m_2 | j_1 j_2 j_{12} m_{12}\rangle \tag{2.36}$$

Eqs. (2.35) and (2.36) together give

$$\begin{aligned} |\gamma(j_1 j_2) j_{12} j_3 JM\rangle = & \sum_{m_{12} m_3 m_1 m_2} |\gamma j_1 j_2 j_3 m_1 m_2 m_3\rangle \times \\ & \langle j_1 j_2 m_1 m_2 | j_1 j_2 j_{12} m_{12}\rangle \langle (j_1 j_2) j_{12} j_3 m_{12} m_3 | (j_1 j_2) j_{12} j_3 JM\rangle \end{aligned} \tag{2.37}$$

and for Eq.(2.33)

$$\begin{aligned} |\gamma j_1 (j_2 j_3) j_{23} JM\rangle = & \sum_{m_{23} m_1 m_2 m_3} |\gamma j_1 j_2 j_3 m_1 m_2 m_3\rangle \times \\ & \langle j_2 j_3 m_2 m_3 | j_2 j_3 j_{23} m_{23}\rangle \langle j_1 (j_2 j_3) j_{23} m_1 m_{23} | j_1 (j_2 j_3) j_{23} JM\rangle \end{aligned} \tag{2.38}$$

It has already been pointed out that both sets Eqs. (2.32) and (2.33) are complete and orthonormal, hence we can change representation , *i.e.*

$$|\gamma j_1 (j_2 j_3) j_{23} JM\rangle = \sum_{j_{12}} |\gamma(j_1 j_2) j_{12} j_3 JM\rangle \langle (j_1 j_2) j_{12} j_3 J | j_1 (j_2 j_3) j_{23} J\rangle \tag{2.39}$$

Note that the summation is only over j_{12} because all other quantum numbers are shared. Also note that the expansion coefficients in Eq. (2.39) is independent of γ and M and these are therefore left out. Eqs. (2.37) and (2.38) when orthogonality and the definition of $3j$-symbols (Eq. (2.16)) has been used, gives (*c.f.* Eq. (2.4) and Eq. (2.5)) for the overlap in Eq. (2.39)

$$
\begin{aligned}
&\langle (j_1 j_2) j_{12} j_3 J | j_1 (j_2 j_3) j_{23} J \rangle = \int d\bar{r} \Phi(\gamma (j_1 j_2) j_{12} j_3 JM)^* \Phi(\gamma j_1 (j_2 j_3) j_{23} JM) \\
= & \sum_{m_1 m_2 m_3 m_{12} m_{23}} \langle j_1 j_2 m_1 m_2 | j_1 j_2 j_{12} m_{12} \rangle \langle j_{12} j_3 m_{12} m_3 | j_{12} j_3 JM \rangle \\
\times & \langle j_2 j_3 m_2 m_3 | j_2 j_3 j_{23} m_{23} \rangle \langle j_1 j_{23} m_1 m_{23} | j_1 j_{23} JM \rangle \\
= & \sum_{m_1 m_2 m_3 m_{12} m_{23}} (-1)^{j_1 - j_2 + m_{12} + j_{12} - j_3 + M + j_2 - j_3 + m_{23} + j_1 - j_{23} + M} \sqrt{[j_{12}][j_{23}]}[J] \\
\times & \begin{pmatrix} j_1 & j_2 & j_{12} \\ m_1 & m_2 & -m_{12} \end{pmatrix} \begin{pmatrix} j_{12} & j_3 & J \\ m_{12} & m_3 & -M \end{pmatrix} \\
\times & \begin{pmatrix} j_2 & j_3 & j_{23} \\ m_2 & m_3 & -m_{23} \end{pmatrix} \begin{pmatrix} j_1 & j_{23} & J \\ m_1 & m_{23} & -M \end{pmatrix}
\end{aligned} \tag{2.40}
$$

where the symbol $[x] = (2x+1)$ has been used. Now rewrite Eq. (2.40) as

$$
\langle (j_1 j_2) j_{12} j_3 J | j_1 (j_2 j_3) j_{23} J \rangle = (-1)^{j_1 + j_2 + j_3 + J} \begin{Bmatrix} j_1 & j_2 & j_{12} \\ j_3 & J & j_{23} \end{Bmatrix} \tag{2.41}
$$

Note that the left hand side of Eq. (2.40) is independent of M and we can therefore replace $[J] = (2J+1)$ with a summation over M and Eq. (2.41) together with Eq. (2.40) give the following symmetric expression for the $6j$-symbol

$$
\begin{aligned}
&\begin{Bmatrix} j_1 & j_2 & j_3 \\ j_4 & j_5 & j_6 \end{Bmatrix} = \\
&\sum_{m_1 m_2 m_3 m_4 m_5 m_6} (-1)^{j_4 + j_5 + j_6 + m_4 + m_5 + m_6} \begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix} \times \\
&\begin{pmatrix} j_1 & j_5 & j_6 \\ m_1 & m_5 & -m_6 \end{pmatrix} \begin{pmatrix} j_4 & j_2 & j_6 \\ -m_4 & m_2 & m_6 \end{pmatrix} \begin{pmatrix} j_4 & j_5 & j_3 \\ m_4 & -m_5 & m_3 \end{pmatrix}
\end{aligned} \tag{2.42}
$$

As we have seen before, the $3j$-symbols put restrictions on the j-values and therefore we have the following triangular conditions that must be satisfied for the $6j$-symbol to be non-zero ($\Delta(j_1 j_2 j_3)$, $\Delta(j_1 j_5 j_6)$, $\Delta(j_4 j_2 j_6)$ and $\Delta(j_4 j_5 j_3)$, respectively)

$$
\left\{ \begin{array}{ccc} - & - & - \\ & & \end{array} \right\}, \left\{ \begin{array}{ccc} \backslash & & \\ & - & - \end{array} \right\}, \left\{ \begin{array}{ccc} & - & \\ / & & \backslash \end{array} \right\}, \left\{ \begin{array}{ccc} & & / \\ - & - & \end{array} \right\} \tag{2.43}
$$

or as a figure (see figure **??**). fig3.

Two useful properties that the $6j$-symbol possess are

i) The $6j$-symbol is invariant under any permutation of its columns, *e.g.*

$$
\begin{Bmatrix} j_1 & j_2 & j_3 \\ j_4 & j_5 & j_6 \end{Bmatrix} = \begin{Bmatrix} j_2 & j_1 & j_3 \\ j_5 & j_4 & j_6 \end{Bmatrix} \tag{2.44}
$$

ii) The $6j$-symbol is invariant under interchange of any two arguments in the columns, *e.g.*

$$\left\{ \begin{matrix} j_1 & j_2 & j_3 \\ j_4 & j_5 & j_6 \end{matrix} \right\} = \left\{ \begin{matrix} j_4 & j_2 & j_6 \\ j_1 & j_5 & j_3 \end{matrix} \right\} \tag{2.45}$$

We also note that the $6j$-symbol is related to the less symmetric Racah coefficient by

$$\left\{ \begin{matrix} j_1 & j_2 & j_3 \\ j_4 & j_5 & j_6 \end{matrix} \right\} = (-1)^{j_1+j_2+j_4+j_5} W(j_1 j_2 j_5 j_4; j_3 j_6) \tag{2.46}$$

To summarize the $6j$-symbol section we note that the $6j$-symbol appeared when re-coupling three angular momenta. Just adding j_1, j_2 and j_3 to form J was not good enough and we had to specify an intermediate state j_{12}, j_{23} or j_{13}. The eigenkets in these two representations are denoted

$$\left. \begin{matrix} |\gamma(j_1 j_2) j_{12} j_3 JM\rangle \\ |\gamma j_1 (j_2 j_2) j_{23} JM\rangle \end{matrix} \right\} \tag{2.47}$$

and the $6j$-symbol is defined by the overlap of these two kets (different representations)

$$\langle (j_1 j_2) j_{12} j_3 J | j_1 (j_2 j_3) j_{23} J \rangle \propto \left\{ \begin{matrix} j_1 & j_2 & j_{12} \\ j_3 & J & j_{23} \end{matrix} \right\} \tag{2.48}$$

the $6j$-symbol appears extensively in the calculation of reduced matrix elements of tensor operators, more on that later.

2.4.2 The 9j-symbol

When coupling four angular momenta, two intermediate states has to be specified for the states to be uniquely defined. To illustrate this we look at figure **??**.

fig4.

The eigenkets in the two representations can be written

$$|\gamma(j_1 j_2) j_{12} (j_3 j_4) j_{34} JM\rangle \tag{2.49}$$

$$|\gamma(j_1 j_3) j_{13} (j_2 j_4) j_{24} JM\rangle \tag{2.50}$$

As was done in Eq. (2.39) we can change between the two representations, both sets are complete and orthonormal. We write this

$$\begin{aligned} |\gamma(j_1 j_3) j_{13} (j_2 j_4) j_{24} JM\rangle &= \sum_{j_{12} j_{34}} |\gamma(j_1 j_2) j_{12} (j_3 j_4) j_{34} JM\rangle \times \\ &\langle (j_1 j_2) j_{12} (j_3 j_4) j_{34} J | (j_1 j_3) j_{13} (j_2 j_4) j_{24} J \rangle \end{aligned} \tag{2.51}$$

and because the expansion coefficients are independent of γ and M these are not shown. The change of representation Eq. (2.51) can be done in three steps, each step involving only three vectors thus allowing us to use the formalism developed in the precious section.

First consider j_3 and j_4 as constant and therefore fixed coupled to j_{34}. To study the coupling between j_1, j_2 and j_{34} forming J we can chose to study $(j_1j_2)j_{12}$ or $(j_2j_{34})j_{324}$ and we get using Eq. (2.39) applied on Eq. (2.49)

$$\begin{aligned}|(\gamma j_3j_4)(j_1j_2)j_{12}j_{34}JM\rangle &= \sum_{j_{234}} |(\gamma j_3j_4)j_1(j_2j_{34})j_{234}JM\rangle \times \\ &\langle j_1(j_2j_{34})j_{234}J|(j_1j_2)j_{12}j_{34}J\rangle \end{aligned} \tag{2.52}$$

As usually we have dropped unnecessary quantum numbers in the coupling coefficients. Also note that j_3 and j_4 have been written together with γ because these are here constant. Standard vector coupling on the ket on the right hand side in Eq. (2.52) give for the same equation

$$\begin{aligned}|(\gamma j_3j_4)(j_1j_2)j_{12}j_{34}JM\rangle &= \sum_{j_{234}m_1m_{234}} |(\gamma j_2j_3j_4j_{34})j_1j_{234}m_1m_{234}\rangle \times \\ &\langle j_1(j_2j_{34})j_{234}J|(j_1j_2)j_{12}j_{34}J\rangle\langle j_1j_{234}m_1m_{234}|j_1j_{234}JM\rangle \end{aligned} \tag{2.53}$$

The corresponding expression for Eq. (2.50) is

$$\begin{aligned}|(\gamma j_2j_4)(j_1j_3)j_{13}j_{24}JM\rangle &= \sum_{j'_{234}m'_1m'_{234}} |(\gamma j_2j_3j_4j_{24})j_1j'_{234}m'_1m'_{234}\rangle \times \\ &\langle j_1(j_3j_{24})j'_{234}J|(j_1j_3)j_{13}j_{24}J\rangle\langle j_1j'_{234}m'_1m'_{234}|j_1j'_{234}JM\rangle \end{aligned} \tag{2.54}$$

We also note that the transformation between $j_3(j_2j_4)j_{24}$ and $(j_3j_4)j_{34}j_2$ is

$$\begin{aligned}|(\gamma j_1j_{234}m_1m_{234})j_3(j_2j_4)j_{24}\rangle &= \sum_{j_{34}} |(\gamma j_1j_{234}m_1m_{234})(j_3j_4)j_{34}j_2\rangle \times \\ &\langle (j_3j_4)j_{34}j_2j_{234}|j_3(j_2j_4)j_{24}j_{234}\rangle \end{aligned} \tag{2.55}$$

Eq. (2.55) tell us how to get between the representations used on the right hand side of Eqs. (2.53) and (2.54).

The coupling coefficient (overlap) in Eq. (2.51) can now be written, using Eqs. (2.53), (2.54) and (2.55)

$$\begin{aligned}&\langle (j_1j_2)j_{12}(j_3j_4)j_{34}J|(j_1j_3)j_{13}(j_2j_4)j_{24}J\rangle = \int d\bar{r}\Phi^*(\ldots)\Phi(\ldots) = \\ &\sum_{j_{234}}\langle (j_1j_2)j_{12}j_{34}J|j_1(j_2j_{34})j_{234}J\rangle\langle (j_3j_4)j_{34}j_2j_{234}|j_3(j_2j_4)j_{24}j_{234}\rangle \times \\ &\langle j_1(j_3j_{24})j_{234}J|(j_1j_3)j_{13}j_{24}J\rangle \end{aligned} \tag{2.56}$$

where we have used the following

$$\langle (\gamma j_2j_3j_4j_{34})j_1j_{234}m_1m_{234}|(\gamma j_2j_3j_4j_{24})j_1j'_{234}m'_1m'_{234}\rangle = \tag{2.57}$$

$$\sum_{j_{34}}\langle (j_3j_4)j_{34}j_2j_{234}|j_3(j_2j_4)j_{24}j_{234}\rangle\delta_{j'_{234}j_{324}}\delta_{m'_1m_1}\delta_{m'_{234}m_{234}} \tag{2.58}$$

$$\sum_{m'_1m'_{234}} |\ldots m'_1m'_{324}\rangle\langle\ldots m'_1m'_{324}| = 1 \tag{2.59}$$

and

$$\langle A|A\rangle = 1 \tag{2.60}$$

The sums over j_{34} in Eq. (2.58) can now be removed because j_3 and j_4 are not fixed coupled to j_{34} in Eq. (2.56). By using the results in Eq. (2.41), Eq. (2.56) takes the form

$$\begin{aligned}&\langle (j_1j_2)j_{12}(j_3j_4)j_{34}J|(j_1j_3)j_{13}(j_2j_4)j_{24}J\rangle = \sqrt{[j_{12}][j_{34}][j_{13}][j_{24}]}\times\\ &\sum_{j_{234}}(-1)^{2j_{234}}[j_{234}]\left\{\begin{array}{ccc} j_1 & j_2 & j_{12}\\ j_{34} & J & j_{234}\end{array}\right\}\left\{\begin{array}{ccc} j_3 & j_4 & j_{34}\\ j_2 & j_{234} & j_{24}\end{array}\right\}\left\{\begin{array}{ccc} j_1 & j_3 & j_{13}\\ j_{24} & J & j_{234}\end{array}\right\}\end{aligned} \tag{2.61}$$

and with the above equation in mind the $9j$-symbol is naturally defined by

$$\langle (j_1j_2)j_{12}(j_3j_4)j_{34}J|(j_1j_3)j_{13}(j_2j_4)j_{24}J\rangle = \sqrt{[j_{12}][j_{34}][j_{13}][j_{24}]}\left\{\begin{array}{ccc} j_1 & j_2 & j_{12}\\ j_3 & j_4 & j_{34}\\ j_{13} & j_{24} & J\end{array}\right\} \tag{2.62}$$

Eqs. (2.61) and (2.62) relate the $9j$- and $6j$-symbols

$$\left\{\begin{array}{ccc} j_1 & j_2 & j_3\\ j_4 & j_5 & j_6\\ j_7 & j_8 & j_9\end{array}\right\} = \sum_x(-1)^{2x}[x]\left\{\begin{array}{ccc} j_1 & j_4 & j_7\\ j_8 & j_9 & x\end{array}\right\}\left\{\begin{array}{ccc} j_2 & j_5 & j_8\\ j_4 & x & j_6\end{array}\right\}\left\{\begin{array}{ccc} j_3 & j_6 & j_9\\ x & j_1 & j_2\end{array}\right\} \tag{2.63}$$

Maybe the most common application for the $9j$-symbol is when changing representation from LS- to jj-coupling in a system of two equivalent electrons, *e.g.*
fig 5.
Changing from jj- to LS-coupling (illustrated in figure **??**) lead to

$$\begin{aligned}&|\gamma(s_1l_1)j_1(s_2l_2)j_2JM\rangle = \sum_{SL}|\gamma(s_1s_2)S(l_1l_2)LJM\rangle\times\\ &\langle (s_1s_2)S(l_1l_2)LJ|(s_1l_1)j_1(s_2l_2)j_2J\rangle = \\ &\sum_{SL}|\gamma(s_1s_2)S(l_1l_2)LJM\rangle\sqrt{[S][L][j_1][j_2]}\left\{\begin{array}{ccc} s_1 & s_2 & S\\ l_1 & l_2 & L\\ j_1 & j_2 & J\end{array}\right\}\end{aligned} \tag{2.64}$$

It is straight forward to obtain the relation between $9j$- and $3j$-symbols, *c.f.* Eq. (2.63) where the relation between $9j$- and $6j$-symbols were derived. Pairwise decoupling of the momenta, *i.e.* first decouple j_{12} and j_{34} from J and then j_1 and j_2 from j_{12} and finally j_3 and j_4 from j_{34}. We get

$$\begin{aligned}&|\gamma(j_1j_2)j_{12}(j_3j_4)j_{34}JM\rangle = \sum_{m_1m_2m_3m_4m_{12}m_{34}}|\gamma j_1j_2j_3j_4m_1m_2m_3m_4\rangle\times\\ &\langle j_1j_2m_1m_2|j_1j_2j_{12}m_{12}\rangle\langle j_3j_4m_3m_4|j_3j_4j_{34}m_{34}\rangle\langle j_{12}j_{34}m_{12}m_{34}|j_{12}j_{34}JM\rangle\end{aligned} \tag{2.65}$$

and

$$\begin{aligned}&|\gamma(j_1j_3)j_{13}(j_2j_4)j_{24}JM\rangle = \sum_{m_1m_2m_3m_4m_{13}m_{24}}|\gamma j_1j_2j_3j_4m_1m_2m_3m_4\rangle\times\\ &\langle j_1j_3m_1m_3|j_1j_3j_{13}m_{13}\rangle\langle j_2j_4m_2m_4|j_2j_4j_{24}m_{24}\rangle\langle j_{13}j_{24}m_{13}m_{24}|j_{13}j_{24}JM\rangle\end{aligned} \tag{2.66}$$

In changing representation from that of Eq. (2.66) to that of Eq. (2.65) involves Eq. (2.51) where once again (*c.f.* Eq. (2.56)) we are interested in the coupling coefficient (overlap). This all together give for the overlap (the summations are over $m_1 m_2 m_3 m_4 m_{12} m_{34} m_{13} m_{24}$)

$$\begin{aligned}
&\langle (j_1 j_2) j_{12} (j_3 j_4) j_{34} J | (j_1 j_3) j_{13} (j_2 j_4) j_{24} J \rangle = \\
&\sum \langle j_{12} j_{34} JM | j_{12} j_{34} m_{12} m_{34} \rangle \langle j_3 j_4 j_{34} m_{34} | j_3 j_4 m_3 m_4 \rangle \langle j_1 j_2 j_{12} m_{12} | j_1 j_2 m_1 m_2 \rangle \times \\
&\langle j_1 j_3 m_1 m_3 | j_1 j_3 j_{13} m_{13} \rangle \langle j_2 j_4 m_2 m_4 | j_2 j_4 j_{24} m_{24} \rangle \langle j_{13} j_{24} m_{13} m_{24} | j_{13} j_{24} JM \rangle = \\
&\sum (-1)^{j_{12}-j_{34}+M+j_3-j_4+m_{34}+j_1-j_2+m_{12}+j_1-j_3+m_{13}+j_2-j_4+m_{24}+j_{13}-j_{24}+M} \times \\
&[J]\sqrt{[j_{12}][j_{34}][j_{13}][j_{24}]} \begin{pmatrix} j_{12} & j_{34} & J \\ m_{12} & m_{34} & -M \end{pmatrix} \begin{pmatrix} j_3 & j_4 & j_{34} \\ m_3 & m_4 & -m_{34} \end{pmatrix} \times \\
&\begin{pmatrix} j_1 & j_2 & j_{12} \\ m_1 & m_2 & -m_{12} \end{pmatrix} \begin{pmatrix} j_1 & j_3 & j_{13} \\ m_1 & m_3 & -m_{13} \end{pmatrix} \begin{pmatrix} j_2 & j_4 & j_{24} \\ m_2 & m_4 & -m_{24} \end{pmatrix} \times \\
&\begin{pmatrix} j_{13} & j_{24} & J \\ m_{13} & m_{24} & -M \end{pmatrix} = \sqrt{[j_{12}][j_{34}][j_{13}][j_{24}]} \begin{Bmatrix} j_1 & j_2 & j_{12} \\ j_3 & j_4 & j_{34} \\ j_{13} & j_{24} & J \end{Bmatrix}
\end{aligned} \tag{2.67}$$

Once again noting that the expression is independent of M which means that we can replace $[J]$ by a sum over M. Finally after this rather tedious procedure, we can write down the relation between $9j$- and $3j$-symbols,

$$\begin{Bmatrix} j_1 & j_2 & j_3 \\ j_4 & j_5 & j_6 \\ j_7 & j_8 & j_9 \end{Bmatrix} = \sum_{m_1,\dots,m_9} \begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix} \begin{pmatrix} j_4 & j_5 & j_6 \\ m_4 & m_5 & m_6 \end{pmatrix} \times \tag{2.68}$$

$$\begin{pmatrix} j_7 & j_8 & j_9 \\ m_7 & m_8 & m_9 \end{pmatrix} \begin{pmatrix} j_1 & j_4 & j_7 \\ m_1 & m_4 & m_7 \end{pmatrix} \begin{pmatrix} j_2 & j_5 & j_8 \\ m_2 & m_5 & m_8 \end{pmatrix} \begin{pmatrix} j_3 & j_6 & j_9 \\ m_3 & m_6 & m_9 \end{pmatrix} \tag{2.69}$$

From the symmetry properties of $3j$-symbols it follows that the arguments in each row/column must satisfy the triangular condition, see Eq. (2.23). An odd permutation of rows/columns change sign on the $9j$-symbol if $\sum_i j_i$ is odd, and the $9j$-symbol is invariant under an even permutation. Later on it will show very useful to know how the $9j$-symbol behave when one of its arguments is zero. We start by noting that

$$\begin{pmatrix} j & j & 0 \\ m & -m & 0 \end{pmatrix} = (-1)^{j-m}([j])^{-1/2} \tag{2.70}$$

This together with the definitions of $9j$- and $6j$-symbols in terms of $3j$-symbols (Eqs. (2.69) and (2.42), respectively) give

$$\begin{Bmatrix} j_1 & j_2 & j_3 \\ j_4 & j_5 & j_3 \\ j_7 & j_7 & 0 \end{Bmatrix} = (-1)^{j_2+j_4+j_3+j_7}([j_3][j_7])^{-1/2} \begin{Bmatrix} j_1 & j_2 & j_3 \\ j_5 & j_4 & j_7 \end{Bmatrix} \tag{2.71}$$

Note that $j_6 = j_3$ and $j_8 = j_7$ because of the triangular condition.

We finish the $9j$-symbol section by remarking that the $9j$-symbol is important not only when going from LS- to jj-coupling but also when calculating matrix elements of tensor products as will be recognized later.

2.4.3 The 12j-symbol

When re-coupling five angular momenta we will encounter the $12j$-symbol. Because the number of indexes have increased we now use letters to mark the angular momenta. The overlap elements when changing coupling schemes from

$$a+b=e,\ r+e=p,\ c+d=f,\ p+f=s \tag{2.72}$$

to (by permuting $b,\ c$)

$$a+c=g,\ r+g=q,\ b+d=h,\ h+q=s \tag{2.73}$$

when the five angular momenta a, b, c, d and r shall be added to form s, and we have to specify the intermediate states c, p, f and g, q, h for the two different representations, is:

$$\langle (r(ab)e)p(cd)fs|(r(ac)g)q(bd)hs\rangle = \sqrt{[e][f][g][h][p][q]}\left\{\begin{matrix} a & b & e & p \\ c & d & f & q \\ g & h & r & s \end{matrix}\right\} \tag{2.74}$$

The relation of $12j$- to $9j$- and $6j$-symbols is

$$\begin{aligned}
&\left\{\begin{matrix} a & b & e & p \\ c & d & f & q \\ g & h & r & s \end{matrix}\right\} = \\
&(-1)^{e+f+g+h}\sum_x (-1)^{2x}[x]\left\{\begin{matrix} a & b & e \\ c & d & f \\ g & h & x \end{matrix}\right\}\left\{\begin{matrix} r & e & p \\ f & s & x \end{matrix}\right\}\left\{\begin{matrix} r & g & q \\ h & s & x \end{matrix}\right\} = \\
&(-1)^{t}\sum_x (-1)^{-x}[x]\left\{\begin{matrix} b & c & x \\ g & e & a \end{matrix}\right\}\left\{\begin{matrix} g & e & x \\ p & q & r \end{matrix}\right\}\left\{\begin{matrix} p & q & x \\ h & f & s \end{matrix}\right\}\left\{\begin{matrix} h & f & x \\ c & b & d \end{matrix}\right\}
\end{aligned} \tag{2.75}$$

t is the sum of all angular momenta in the $12j$-symbol. The $12j$-symbols are used when calculating the fractional parentage coefficients to which we will return later.